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Recent Advances in Achieving Textbook Multigrid Efficiency for Computational Fluid Dynamics Simulations

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RECENT ADVANCES IN ACHIEVING TEXTBOOK MULTIGRID EFFICIENCY FOR COMPUTATIONAL FLUID DYNAMICS SIMULATIONS

ACHI BRANDT*, BORIS DISKIN†, AND JAMES L. THOMAS‡

Abstract. Recent advances in achieving textbook multigrid efficiency for fluid simulations are presented. Textbook multigrid efficiency is defined as attaining the solution to the governing system of equations in a computational work which is a small multiple of the operation counts associated with discretizing the system. Strategies are reviewed to attain this efficiency by exploiting the factorizability properties inherent to a range of fluid simulations, including the compressible Navier-Stokes equations. Factorizability is used to separate the elliptic and hyperbolic factors contributing to the target system; each of the factors can then be treated individually and optimally. Boundary regions and discontinuities are addressed with separate (local) treatments. New formulations and recent calculations demonstrating the attainment of textbook efficiency for aerodynamic simulations are shown.

Key words. textbook multigrid efficiency, factorizable systems of differential equations, principal linearization, factorizable discretizations, distributed relaxation

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1. Introduction. Considerable progress over the past thirty years has been made in the development of large-scale computational fluid dynamics (CFD) solvers for the Euler and Navier-Stokes equations. Computations are used routinely to design the cruise shapes of transport aircraft through complex-geometry simulations involving the solution of 25-100 million equations; in this arena, the number of wind-tunnel tests for a new design has been substantially reduced. However, simulations of the entire flight envelope of the vehicle, including maximum lift, buffet onset, flutter, and control effectiveness, have not been as successful in eliminating the reliance on wind-tunnel testing. These simulations involve unsteady flows with more separation and stronger shock waves than at cruise. The main reasons limiting further inroads of CFD into the design process are: (1) the reliability of turbulence models and (2) the time and expense of the numerical simulation. Because of the prohibitive resolution requirements of direct simulations at high Reynolds numbers, transition and turbulence modeling is expected to remain an issue for the near term [41]. The focus of this paper addresses the latter problem by attempting to attain optimal efficiencies in solving the governing equations. Typically current CFD codes based on the use of multigrid acceleration techniques and multistage Runge-Kutta time-stepping schemes are able to converge lift and drag values for cruise configurations within approximately 1000 residual evaluations. More complexity in the geometry or physics generally requires many more residual evaluations to converge, and sometimes convergence cannot be attained. An optimally convergent method is defined [5, 6, 8, 9] as having textbook multigrid efficiency (TME), meaning the solutions to the governing system of equations are attained in a computational work which is a small (less than 10) multiple of the operation count in the discretized system of equations (residual evaluations).

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Thus, there is a potential gain of more than two orders of magnitude in operation count reduction if TME could be attained. For staggered-grid formulations of incompressible flow equations, robust and relatively efficient multigrid solvers have already been developed [30, 31, 32]; their efficiency is still about an order of magnitude behind TME.

Because the governing equations are a set of coupled nonlinear conservation equations with discontinuities (shocks, slip lines, etc.) and singularities (flow- or grid-induced), the difficulties are numerous. The TME methodology insists that each of the difficulties should be isolated, analyzed, and solved systematically using a carefully constructed series of model problems. To be efficient, multigrid solvers for general systems of partial differential equations must adequately address three types of errors: (1) high-frequency error components, (2) uniformly smooth error components, and (3) characteristic error components. The latter are (usually smooth) error components that are much smoother in characteristic directions than in other directions. Standard multigrid methods that are efficient for elliptic problems recognize and separate the treatment of high-frequency and smooth error components. The former are efficiently reduced in relaxation; the latter are well approximated on coarse grids and, hence, eliminated through the coarse-grid correction. The efficiency of classical multigrid methods severely degrades for nonelliptic problems because characteristic components cannot be adequately approximated on coarse grids [4, 11, 15].

If the target discretization is h -elliptic (or semi- h -elliptic), the high frequency error components can still be reduced by a local (or block-wise) relaxation procedure. By definition [4, 55], a discrete scalar (not necessarily elliptic) operator $L[u]$ possesses a good measure of h -ellipticity if the absolute value of its symbol $|L(\bar{\theta})| = |e^{-i(\bar{\theta} \cdot \mathbf{j})} L[e^{i(\bar{\theta} \cdot \mathbf{j})}]|$ is well separated from zero for all high-frequency Fourier modes. Here $\mathbf{j} = (j_x, j_y, j_z)$ are the grid indexes and $\bar{\theta} = (\theta_x, \theta_y, \theta_z)$, $0 \leq |\theta_x|, |\theta_y|, |\theta_z| \leq \pi$ are normalized Fourier frequencies. High-frequency Fourier modes are the modes satisfying $\max(|\theta_x|, |\theta_y|, |\theta_z|) \geq \frac{\pi}{2}$. For systems, the measure of h -ellipticity is defined as the absolute value of the determinant of the operator matrix.

Standard coarse-grid corrections are efficient for uniformly smooth error components, even for nonelliptic problems. An effective reduction of characteristic error components can be achieved either by designing a proper relaxation scheme reducing not only high-frequency but smooth error components as well (e.g., by downstream ordering of relaxation steps) or by adjusting coarse-grid operators for a better characteristic-component approximation.

Multigrid methods efficiently reducing all the three aforementioned types of error have been developed for *scalar* nonelliptic operators [11, 12, 20, 21, 22]. TME for *systems* of equations can be attained by exploiting the factorizability property of the governing equations. The factorizability of the Navier-Stokes equations is manifested by the fact that the determinant of the matrix of the differential operators consists of separable factors. Exploiting the factorizability property in discrete computations reduces the problem of relaxing a complicated system of discretized coupled differential equations to relaxation of simpler factors constituting the system determinant. This approach is quite distinct from most approaches to accelerate convergence because for steady-state flows, the factors are treated directly rather than through pseudo-time marching methods. Time-dependent flow solvers can be constructed within this approach as well and in principle are simpler to develop than steady-state solvers. A list of envisioned difficulties and possible solutions in attaining TME for CFD simulations is discussed elsewhere [9].

This paper is organized as follows. The foundations of the methodology for attaining TME in CFD simulations are discussed in Section 2, including the concept of principal linearization and illustrations of the factorizability of various fluid dynamic equations. Two strategies for exploiting the factorizability are presented in the next two sections. Reformulation of the differential equations is discussed in Section 3. An

alternative, more general, distributed relaxation approach is discussed in Section 4. Efficient methods for relaxing scalar factors are presented in Section 5. Section 6 compares and evaluates the available analytical tools. Section 7 summarizes recent advances in formulation and demonstration TME. Concluding remarks are given in the final Section 8.

2. Foundations for Textbook Multigrid Efficiency. The basic framework for TME solvers is full multigrid (FMG) algorithms [5, 6, 17, 46, 55, 56]. In FMG algorithms, the solution process is started on a very coarse grid where the computational cost of solution is negligible. The coarse-grid solution is then interpolated to the next fine grid to form an initial approximation. Few multigrid full approximation scheme (FAS) cycles, or possibly just one, are performed next to obtain an improved fine-grid solution approximation. Then, the process proceeds to finer grids until the solution on the target finest grid is achieved.

In the solution of highly nonlinear problems, a good initial guess is important. A general way to obtain such an initial guess is by continuation, in which the solution to the target problem is approached through the solutions of a sequence of parameterized problems. Usually the problem starting the continuation process is easy to solve, and the difficulty gradually increases as the control parameter approaches the target value; this continuation process can often be integrated into an FMG solver. For example, with viscosity as the control parameter, at the coarse grids more artificial viscosity can be used, then gradually be taken out as the algorithm proceeds to finer levels. Such FMG continuation is often natural because larger numerical viscosity is introduced on coarse grids, even without aiming at continuation.

A version named λ -FMG algorithm provides the device needed for optimal adaptive local refinement. Efficient multigrid solvers based on this approach have been demonstrated [2].

The objective of FMG algorithms (and TME methods in particular) is fast convergence to the solution of the differential equations, not necessarily fast asymptotic residual convergence. The natural solution tolerance is the discretization error defined as the difference between the exact solutions of discrete and differential problems. Thus, the quality of a solution approximation on a given grid can be measured by the relative magnitude of algebraic errors in comparison with the discretization error level. The algebraic error is defined as the difference between the exact and approximate solutions of the discrete problem. On any grid in an FMG algorithm, we expect the algebraic errors after few multigrid cycles to be always less than the discretization error.

On the other hand, a fast residual convergence is considered as an important monitoring tool. In many practical cases, it is possible to develop a solver exhibiting fast residual convergence rates without compromising TME. Note however that sometimes the quality of the target-grid solution can be much improved by double discretization methods. A double discretization method applies for relaxation a discretization scheme that is different from the scheme used for calculating residuals transferred to the coarse grid. Zero target-grid residuals might not be the aim in this case.

The goal of this paper is to review solution strategies leading to TME solution of fluid mechanics equations. The most general system we consider here is the time-dependent compressible Navier-Stokes equations written as

$$(2.1) \quad \partial_t \mathbf{Q} + \mathbf{R}(\mathbf{Q}) = 0,$$

where the conserved variables are $\mathbf{Q} \equiv (\rho u, \rho v, \rho w, \rho, \rho E)^T$, representing the momentum vector, density, and total energy per unit volume, and

$$(2.2) \quad \mathbf{R}(\mathbf{Q}) \equiv \partial_x \mathbf{F}(\mathbf{Q}) + \partial_y \mathbf{G}(\mathbf{Q}) + \partial_z \mathbf{H}(\mathbf{Q}),$$

$$\begin{aligned}
\mathbf{F}(\mathbf{Q}) &= \begin{pmatrix} \rho u^2 + p - 2\mu\partial_x u - \lambda(\nabla \cdot \mathbf{u}) \\ \rho uv - \mu(\partial_x v + \partial_y u) \\ \rho uw - \mu(\partial_x w + \partial_z u) \\ \rho u \\ \rho u E + up - \lambda u(\nabla \cdot \mathbf{u}) - \mu\tau_1 - \kappa\partial_x \epsilon \end{pmatrix}, \\
\mathbf{G}(\mathbf{Q}) &= \begin{pmatrix} \rho uv - \mu(\partial_x v + \partial_y u) \\ \rho v^2 + p - 2\mu\partial_y v - \lambda(\nabla \cdot \mathbf{u}) \\ \rho vw - \mu(\partial_y w + \partial_z v) \\ \rho v \\ \rho v E + vp - \lambda v(\nabla \cdot \mathbf{u}) - \mu\tau_2 - \kappa\partial_y \epsilon \end{pmatrix}, \\
\mathbf{H}(\mathbf{Q}) &= \begin{pmatrix} \rho uw - \mu(\partial_x w + \partial_z u) \\ \rho vw - \mu(\partial_y w + \partial_z v) \\ \rho w^2 + p - 2\mu\partial_z w - \lambda(\nabla \cdot \mathbf{u}) \\ \rho w \\ \rho w E + wp - \lambda w(\nabla \cdot \mathbf{u}) - \mu\tau_3 - \kappa\partial_z \epsilon \end{pmatrix},
\end{aligned}$$

where

$$\begin{aligned}
\tau_1 &= 2u\partial_x u + v(\partial_x v + \partial_y u) + w(\partial_x w + \partial_z u), \\
\tau_2 &= 2v\partial_y v + u(\partial_x v + \partial_y u) + w(\partial_y w + \partial_z v), \\
\tau_3 &= 2w\partial_z w + u(\partial_x w + \partial_z u) + v(\partial_y w + \partial_z v),
\end{aligned}$$

μ and λ are viscosity coefficients, and κ is the coefficient of heat conductivity.

A basic step in developing an efficient multigrid algorithm is to design an efficient relaxation procedure. For nonlinear problems, the relaxation updates to a current solution approximation are usually computed through Newton iterations. The full Newton linearization of the Navier-Stokes equations (2.1) is a very complicated operator, and its solution (inversion) is too costly for practical applications. To reduce the computational cost without compromising efficiency, one can opt for relaxation of a principal linearization. The principal linearization of a scalar equation contains the linearization terms that make a major contribution to the residual per unit change in the unknown variable. The principal terms thus generally depend on the scale, or mesh size, of interest. For example, the discretized highest derivative terms are principal on grids with small enough mesh size. For a discretized system of differential equations, the principal terms are terms that contribute to the principal terms of the system determinant.

To illustrate the idea of principal linearization, consider a nonlinear discrete thin-layer approximation of the convection-diffusion operator, in which the flow is parallel to the boundary (x -direction) and only the viscous terms associated with variations in the y -coordinate normal to the boundary are retained

$$(2.3) \quad N(u) \equiv u\partial_x^h u - \nu\partial_{yy}^h u,$$

where ∂_x^h and ∂_{yy}^h are discrete approximations to the first x -directional derivative and to the second y -directional derivative, respectively. A full Newton linearization (assuming constant viscosity) for a correction δu has three terms

$$(2.4) \quad \frac{\partial N}{\partial u} \delta u \equiv u\partial_x^h \delta u + (\partial_x^h u)\delta u - \nu\partial_{yy}^h \delta u.$$

To evaluate principality of the terms, one can start from an exact discrete solution; for example, the function $\delta u \equiv 0$ is the exact solution of the homogeneous equation $\frac{\partial N}{\partial u} \delta u = 0$. A unit change in the unknown variable, δu , is defined as a perturbation of the solution value at one grid point. Introducing this perturbation, the residual function becomes nonzero in the vicinity of the perturbed point. One can directly check which of the terms of the full linearization operator make major residual contributions. Three situations are encountered:

- *High cell Reynolds number* ($\frac{uh_y^2}{\nu h_x} \gg 1$). If the velocity function u is smooth and non-degenerate, i.e., the magnitude of velocity deviations in neighboring grid points is less than the local velocity magnitude, then the major contribution to the residual function is $O(u/h_x)$ and comes from the term $u\partial_x^h \delta u$; the second term contribution is $O(\partial_x^h u)$; and the viscous term contributes $O(\nu/h_y^2)$ which is much less than $O(u/h_x)$. Thus, only the first term $u\partial_x^h \delta u$ is principal. However, if the velocity field is not smooth, either because of a coarse mesh or proximity to a discontinuity, or if the absolute velocity value is small (stagnation flows), then the second term becomes principal as well.
- *Low cell Reynolds number* ($\frac{uh_y^2}{\nu h_x} \ll 1$). The major residual contribution comes from the viscous term which is the only principal term.
- *Medium cell Reynolds number* ($\frac{uh_y^2}{\nu h_x} = O(1)$). This situation corresponds to the usual boundary layer assumption when convection balances diffusion. For smooth non-degenerate flows, the only subprincipal term is the second; the first and the third terms are principal. For nonsmooth or degenerate flows, all three terms are principal.

As an example of a system of nonlinear flow equations, we consider a discrete operator corresponding to a one-dimensional steady-state compressible inviscid flow:

$$(2.5) \quad N(\mathbf{q}) \equiv \begin{pmatrix} u\partial_x^h u + \frac{(\gamma-1)\epsilon}{p}\partial_x^h p \\ \gamma p\partial_x^h u + u\partial_x^h p \\ (\gamma-1)\epsilon\partial_x^h u + u\partial_x^h \epsilon \end{pmatrix},$$

where $\mathbf{q} = (u, p, \epsilon)^T$ represents velocity, pressure, and internal energy and γ is the ratio of specific heats. The full Newton linearization of this operator is given by

$$(2.6) \quad \frac{\partial N}{\partial \mathbf{q}} \delta \mathbf{q} \equiv \begin{pmatrix} (\partial_x^h u) + u\partial_x^h & (\gamma-1)\epsilon(\frac{1}{p}\partial_x^h - \frac{(\partial_x^h p)}{p^2}) & (\gamma-1)\frac{(\partial_x^h p)}{p} \\ \gamma p\partial_x^h + (\partial_x^h p) & \gamma(\partial_x^h u) + u\partial_x^h & 0 \\ (\gamma-1)\epsilon\partial_x^h + (\partial_x^h \epsilon) & 0 & (\gamma-1)(\partial_x^h u) + u\partial_x^h \end{pmatrix} \begin{pmatrix} \delta u \\ \delta p \\ \delta \epsilon \end{pmatrix},$$

Assuming a smooth non-degenerate solution \mathbf{q} , the first simplification step is to eliminate lower derivative terms from each entry of the matrix (2.6). This simplification leads to an approximate linearization as

$$(2.7) \quad \begin{pmatrix} u\partial_x^h & (\gamma-1)\frac{\epsilon}{p}\partial_x^h & (\gamma-1)\frac{(\partial_x^h p)}{p} \\ \gamma p\partial_x^h & u\partial_x^h & 0 \\ (\gamma-1)\epsilon\partial_x^h & 0 & u\partial_x^h \end{pmatrix} \begin{pmatrix} \delta u \\ \delta p \\ \delta \epsilon \end{pmatrix},$$

The determinant of the matrix (2.7) is

$$u\partial_x^h (u^2\partial_x^h \partial_x^h - c^2\partial_x^h \partial_x^h - (\gamma-1)^2\frac{\epsilon}{p}(\partial_x^h p)\partial_x^h),$$

where the sound speed c relates to the internal energy ϵ as $c^2 = \gamma(\gamma-1)\epsilon$. Because p is non-degenerate, the last term in the parentheses is subprincipal in comparison to the other two terms. The third element in the first row of the matrix (2.7) does not contribute to the principal part of the determinant operator; therefore the principal linearization is defined as

$$(2.8) \quad \begin{pmatrix} u\partial_x^h & (\gamma-1)\frac{\epsilon}{p}\partial_x^h & 0 \\ \gamma p\partial_x^h & u\partial_x^h & 0 \\ (\gamma-1)\epsilon\partial_x^h & 0 & u\partial_x^h \end{pmatrix} \begin{pmatrix} \delta u \\ \delta p \\ \delta \epsilon \end{pmatrix},$$

The notion of principal linearization is essentially based on the discrete formulation. The principal part of a differential operator may be defined as the limit of the principal part of the corresponding discrete operator as the mesh size h tends to zero. So for smooth non-degenerate flows, the principal terms of the differential equations are the highest derivatives.

TME for solution of the Navier-Stokes system of differential equations can be achieved by exploiting the system factorizability. To illustrate the factorizability property, examples are given below for various fluid mechanics regimes. In all cases, we assume a smooth non-degenerate solution as defined previously.

Incompressible Navier-Stokes Equations. The steady-state incompressible Navier-Stokes equations can be written as

$$(2.9) \quad \begin{aligned} Q_\nu \mathbf{u} + \nabla p &= 0, \\ \nabla \cdot \mathbf{u} &= 0, \end{aligned}$$

where $\mathbf{u} = (u, v, w)^T$ is the velocity vector and $Q_\nu = \mathbf{u} \cdot \nabla - \nu \Delta$ is a convection-diffusion operator. The principal linearization operator is given by

$$(2.10) \quad \mathbf{L} \begin{pmatrix} \delta u \\ \delta v \\ \delta w \\ \delta p \end{pmatrix} = \begin{bmatrix} Q_\nu & 0 & 0 & \partial_x \\ 0 & Q_\nu & 0 & \partial_y \\ 0 & 0 & Q_\nu & \partial_z \\ \partial_x & \partial_y & \partial_z & 0 \end{bmatrix} \begin{pmatrix} \delta u \\ \delta v \\ \delta w \\ \delta p \end{pmatrix},$$

where velocity \mathbf{u} is fixed in the linearized convection-diffusion operator Q_ν .

$$(2.11) \quad \det \mathbf{L} = -Q_\nu^2 \Delta.$$

Compressible Euler Equations. A nonconservative form of the Euler equations is given by

$$\begin{aligned} Q\mathbf{u} + \frac{1}{\rho} \nabla p &= 0, \\ \rho c^2 \nabla \cdot \mathbf{u} + Qp &= 0, \\ \frac{c^2}{\gamma} \nabla \cdot \mathbf{u} + Q\epsilon &= 0, \end{aligned}$$

where $Q \equiv Q_0$ denotes the particular case of Q_ν with zero ($\nu = 0$) physical diffusion, and density, ρ , pressure, p , sound speed, c , and internal energy, ϵ , are related as

$$(2.12) \quad p = (\gamma - 1)\rho\epsilon,$$

$$(2.13) \quad c^2 = \gamma p / \rho.$$

The principal linearization is given by

$$(2.14) \quad \mathbf{L} \begin{pmatrix} \delta u \\ \delta v \\ \delta w \\ \delta p \\ \delta \epsilon \end{pmatrix} = \begin{bmatrix} Q & 0 & 0 & \frac{1}{\rho}\partial_x & 0 \\ 0 & Q & 0 & \frac{1}{\rho}\partial_y & 0 \\ 0 & 0 & Q & \frac{1}{\rho}\partial_z & 0 \\ \rho c^2 \partial_x & \rho c^2 \partial_y & \rho c^2 \partial_z & Q & 0 \\ \frac{c^2}{\gamma} \partial_x & \frac{c^2}{\gamma} \partial_y & \frac{c^2}{\gamma} \partial_z & 0 & Q \end{bmatrix} \begin{pmatrix} \delta u \\ \delta v \\ \delta w \\ \delta p \\ \delta \epsilon \end{pmatrix}.$$

The determinant of the matrix operator \mathbf{L} is

$$(2.15) \quad \det \mathbf{L} = Q^3 [Q^2 - c^2 \Delta],$$

where Δ is the Laplace operator, and $Q^2 - c^2 \Delta$ represents the full-potential operator.

Compressible Navier-Stokes Equations. The nonconservative formulation corresponding to the steady-state version of (2.1) is given by

$$\begin{aligned} & \left((\mathbf{u} \cdot \nabla) - \frac{\mu}{\rho} \Delta - \frac{\hat{\lambda}}{\rho} \partial_{xx} \right) u - \frac{\hat{\lambda}}{\rho} (\partial_{xy} v + \partial_{xz} w) + \frac{1}{\rho} \partial_x p = 0, \\ & \left((\mathbf{u} \cdot \nabla) - \frac{\mu}{\rho} \Delta - \frac{\hat{\lambda}}{\rho} \partial_{yy} \right) v - \frac{\hat{\lambda}}{\rho} (\partial_{xy} u + \partial_{yz} w) + \frac{1}{\rho} \partial_y p = 0, \\ & \left((\mathbf{u} \cdot \nabla) - \frac{\mu}{\rho} \Delta - \frac{\hat{\lambda}}{\rho} \partial_{zz} \right) w - \frac{\hat{\lambda}}{\rho} (\partial_{xz} u + \partial_{yz} v) + \frac{1}{\rho} \partial_z p = 0, \\ & \rho c^2 (\nabla \cdot \mathbf{u}) + (\mathbf{u} \cdot \nabla) p + (\gamma - 1) (-\kappa \Delta \epsilon + \Phi) = 0, \\ & \frac{c^2}{\gamma} (\nabla \cdot \mathbf{u}) + (\mathbf{u} \cdot \nabla) p - \frac{\kappa}{\rho} \Delta \epsilon + \rho \Phi = 0, \end{aligned}$$

where

$$\Phi \equiv \mu \left(2(\partial_x u)^2 + 2(\partial_y v)^2 + 2(\partial_z w)^2 + (\partial_x v + \partial_y u)^2 + (\partial_x w + \partial_z u)^2 + (\partial_y w + \partial_z v)^2 \right) + \lambda (\partial_x u + \partial_y v + \partial_z w)^2.$$

Assuming constant viscosity and heat conduction coefficients, the principal linearization operator \mathbf{L} , keeping the terms principal on both the viscous and inviscid scales, is given by

$$(2.16) \quad \mathbf{L} = \begin{bmatrix} Q \frac{\mu}{\rho} - \frac{\hat{\lambda}}{\rho} \partial_{xx} & -\frac{\hat{\lambda}}{\rho} \partial_{xy} & -\frac{\hat{\lambda}}{\rho} \partial_{xz} & \frac{1}{\rho} \partial_x & 0 \\ -\frac{\hat{\lambda}}{\rho} \partial_{xy} & Q \frac{\mu}{\rho} - \frac{\hat{\lambda}}{\rho} \partial_{yy} & -\frac{\hat{\lambda}}{\rho} \partial_{yz} & \frac{1}{\rho} \partial_y & 0 \\ -\frac{\hat{\lambda}}{\rho} \partial_{xz} & -\frac{\hat{\lambda}}{\rho} \partial_{yz} & Q \frac{\mu}{\rho} - \frac{\hat{\lambda}}{\rho} \partial_{zz} & \frac{1}{\rho} \partial_z & 0 \\ \rho c^2 \partial_x & \rho c^2 \partial_y & \rho c^2 \partial_z & Q & (1 - \gamma) \kappa \Delta \\ \frac{c^2}{\gamma} \partial_x & \frac{c^2}{\gamma} \partial_y & \frac{c^2}{\gamma} \partial_z & 0 & Q \frac{\kappa}{\rho} \end{bmatrix},$$

$$(2.17) \quad \det \mathbf{L} = Q^2 \frac{\mu}{\rho} \left[\frac{\kappa c^2}{\gamma \rho} \Delta^2 + Q (-c^2 \Delta + \frac{\kappa (\hat{\lambda} + \mu)}{\rho^2} \Delta^2) - Q^2 \frac{\kappa + \hat{\lambda} + \mu}{\rho} \Delta + Q^3 \right],$$

where, nondimensionalizing by density and sound speed and applying Stokes hypothesis for the bulk viscosity term, the coefficients become $\mu/\rho = M_\infty/(\rho \text{ Re})$, $\kappa = M_\infty \gamma/(\text{Re Pr})$, and $\hat{\lambda} = \lambda + \mu = \mu/3$; M_∞ is the free stream Mach number, and Re and Pr are Reynolds and Prandtl numbers respectively.

The approaches exploiting the factorizability property for efficient solution of the Navier-Stokes equations may be divided into two categories: (1) reformulating the target differential equations so that the principal linearization of the new formulation becomes uncoupled (usually triangular with the factors of the determinant on the main diagonal) and (2) modifying the equations for computing relaxation updates while keeping the original formulation for computing residuals.

For the subsonic compressible Euler equations, the first TME solvers exploiting factorizability of the system have been developed by Ta'asan [48, 49, 50]. These solvers represent examples of the reformulation approach. New canonical variables have been introduced, and in these variables, the Euler system of equations becomes block upper triangular with the main diagonal blocks consisting of the basic components of the system. Another reformulation approach toward achieving TME for solution of the Euler and incompressible Navier-Stokes equations is based on the pressure-equation formulation which effectively separates elliptic and hyperbolic factors of the system [36, 43, 45].

The approaches from the second category are more general, allowing considerable freedom in relaxation scheme design because different schemes may be applied to different flow regions. However, the design itself is relatively simple only if the target discretization scheme is also factorizable, i.e., the determinant of the discrete principal linearization can be represented as a product of discrete factors, each of them approximating a corresponding factor of the determinant of the differential equations. A stumbling block that has prevented fast progress in developing TME solvers was the lack of factorizable discretizations for many important application areas in fluid mechanics. Among the widely known discretization schemes, only staggered-grid formulations for incompressible and subsonic compressible flow regimes are conveniently factorizable. Some centrally-differenced collocated-grid formulations are factorizable as well, but the factors obtained in the corresponding discrete determinant are not often easily treated. The search for new factorizable discretization schemes (see Summary of Recent Progress below) is chiefly motivated by the need to derive discrete schemes with the resulting discretizations of scalar factors satisfying some desired properties (e.g., stability, correct alignment with the physical anisotropies, compactness, availability of an efficient relaxation scheme, etc.) Development of suitable factorizable discrete schemes for the Navier-Stokes equation is a challenging task. Much of the recent progress in achieving TME for CFD simulations is because new families of general factorizable collocated-grid discretization schemes are emerging [26, 35, 38, 42, 44]. The next two sections present some details of methods from the two categories.

3. Equation Reformulation Strategies. As mentioned previously, the first TME solvers exploiting factorizability of the system have been developed in [48, 49, 50]. The original equations were reformulated in terms of canonical forms, in which the subsystems governed by hyperbolic operators are distinguished and treated separately, both in discretization and relaxation, from those governed by elliptic operators. The canonical variables for two dimensions are velocity (u, v) , entropy s , and total enthalpy H . The elliptic operators are discretized with h -elliptic centered differences and solved with point relaxation and coarse grid corrections; the hyperbolic operators are discretized with upwind schemes and solved by marching techniques. Ta'asan [49] was able to demonstrate solutions for the subsonic compressible Euler equations which converged with the same rates as the solution of the scalar full potential equation. An additional advantage shown for this formulation was that the total artificial viscosity error was smaller than with other schemes because the upwinding was only used for the hyperbolic subsystems. The main disadvantage of this formulation is that it is not easily generalized to viscous and unsteady problems, especially in three dimensions.

An alternative pressure-equation formulation [45] for the incompressible Navier-Stokes equations (2.9) effectively separates the elliptic and hyperbolic factors of the system. The continuity equation is replaced with an equation for the pressure, as

$$(3.1) \quad \nabla(Q_\nu \mathbf{u} + \nabla p) - Q_\nu(\nabla \cdot \mathbf{u}) = 0.$$

Assuming a smooth non-degenerate flow, the principal linearization taken in the limit as mesh size h tends to zero is an upper triangular matrix with the main diagonal composed of the linearized convection-diffusion and Laplace operators,

$$(3.2) \quad \mathbf{L} \equiv \begin{bmatrix} Q_\nu & 0 & 0 & \partial_x \\ 0 & Q_\nu & 0 & \partial_y \\ 0 & 0 & Q_\nu & \partial_z \\ 0 & 0 & 0 & \Delta \end{bmatrix}.$$

The relaxation scheme is defined as

$$(3.3) \quad \mathbf{L}\delta\mathbf{q} = -R(\mathbf{q}),$$

where $R(\mathbf{q})$ is the new nonlinear formulation of the incompressible Navier-Stokes equations.

The determinant of the reformulated system is $Q_\nu^3\Delta$ as compared to $Q_\nu^2\Delta$ of the original system. Thus additional boundary conditions which enforce zero-divergence need to be applied. The equations are uncoupled everywhere except at the boundaries and some local relaxation is needed to relax the equations in this region. Some two-dimensional results are shown subsequently demonstrating the efficiency of this approach. Although unexploited as yet, the approach applies equally well to time-dependent flows. This approach has met difficulties in generalizing to viscous compressible flows.

4. Distributed Relaxation Strategies. The most general procedure exploiting factorizability of the target Navier-Stokes equations is distributed relaxation. The general framework, first introduced in [54] can be outlined as follows.

In general, the simplest form of the differential Navier-Stokes equations corresponds to nonconservative equations expressed in primitive variables, e.g., taken as the set composed of velocity, pressure, and internal energy, $\mathbf{q} = (u, v, w, p, \epsilon)^T$. For a perfect gas, the primitive and conservative variables are connected through (2.12), (2.13), and

$$(4.1) \quad \epsilon = E - \frac{1}{2}(u^2 + v^2 + w^2).$$

The time-dependent nonconservative equations are found readily by transforming the time-dependent conservative equations.

$$\begin{aligned} \frac{\partial \mathbf{q}}{\partial \mathbf{Q}} [\partial_t \mathbf{Q} + \mathbf{R}] &= 0, \\ \partial_t \mathbf{q} + \frac{\partial \mathbf{q}}{\partial \mathbf{Q}} \mathbf{R} &= 0, \end{aligned}$$

where $\frac{\partial \mathbf{q}}{\partial \mathbf{Q}}$ is the Jacobian matrix of the transformation. For steady-state equations, the time derivative is dropped. In an iterative procedure, the correction $\delta\mathbf{q} \equiv \mathbf{q}^{n+1} - \mathbf{q}^n$, where n is an iteration counter, can be computed from the equation

$$(4.2) \quad \mathbf{L}\delta\mathbf{q} = -\frac{\partial \mathbf{q}}{\partial \mathbf{Q}} \mathbf{R},$$

where the right side of (4.2) is a linear combination of the conservative residuals, and \mathbf{L} is the principal linearization of the nonconservative operator at the scale h .

While significantly simplified by retaining only principal terms, the system (4.2) is still a set of coupled equations containing elliptic and hyperbolic components. Therefore, collective Gauss-Seidel relaxation of \mathbf{L}

is not often effective. The distributed relaxation method replaces $\delta \mathbf{q}$ in (4.2) by $\mathbf{M} \delta \mathbf{w}$.

$$(4.3) \quad \mathbf{L} \mathbf{M} \delta \mathbf{w} = -\frac{\partial \mathbf{q}}{\partial \mathbf{Q}} \mathbf{R}.$$

The resulting matrix $\mathbf{L} \mathbf{M}$ becomes lower triangular. The diagonal elements of $\mathbf{L} \mathbf{M}$ are composed ideally of the separable factors of the matrix \mathbf{L} determinant. These factors are scalar differential operators of first or second order, so their efficient relaxation is a much simpler task than relaxing the entire system associated with \mathbf{L} . In relaxing scalar factors, the changes introduced in the “ghost” variables $\delta \mathbf{w}$ (the variables $\delta \mathbf{w}$ are “ghost” because they need not be explicitly used in computations) during relaxation are distributed, with the pattern of the distribution matrix \mathbf{M} , to the primitive variables. To obtain the optimal (textbook) efficiency, relaxation of each factor should incorporate the essential part of an efficient multigrid solver for its corresponding operator: sometimes this essential part is just the relaxation part of that solver, sometimes this may even be an entire separate multigrid solver applied over subdomains.

4.1. Distribution Matrices. For incompressible Navier-Stokes equations, an appropriate distribution matrix corresponding to the operator \mathbf{L} of (3.2) is

$$(4.4) \quad \mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & -\partial_x \\ 0 & 1 & 0 & -\partial_y \\ 0 & 0 & 1 & -\partial_z \\ 0 & 0 & 0 & Q_\nu \end{bmatrix}$$

yielding the lower triangular operator

$$(4.5) \quad \mathbf{L} \mathbf{M} = \begin{bmatrix} Q_\nu & 0 & 0 & 0 \\ 0 & Q_\nu & 0 & 0 \\ 0 & 0 & Q_\nu & 0 \\ \partial_x & \partial_y & \partial_z & -\Delta \end{bmatrix}.$$

A possible distribution matrix for the compressible Euler equations with the principal linearization operator \mathbf{L} (2.14) is given by

$$(4.6) \quad \mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & -\frac{1}{\rho} \partial_x & 0 \\ 0 & 1 & 0 & -\frac{1}{\rho} \partial_y & 0 \\ 0 & 0 & 1 & -\frac{1}{\rho} \partial_z & 0 \\ 0 & 0 & 0 & Q & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

with

$$(4.7) \quad \mathbf{L} \mathbf{M} = \begin{bmatrix} Q & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & 0 & 0 \\ 0 & 0 & Q & 0 & 0 \\ \rho c^2 \partial_x & \rho c^2 \partial_y & \rho c^2 \partial_z & Q^2 - c^2 \Delta & 0 \\ \frac{c^2}{\gamma} \partial_x & \frac{c^2}{\gamma} \partial_y & \frac{c^2}{\gamma} \partial_z & -\frac{c^2}{\rho \gamma} \Delta & Q \end{bmatrix}.$$

For compressible Navier-Stokes equations, one of the factors of the principal-linearization determinant (2.17) is very complicated. Instead of devising a suitable relaxation method for this scalar factor, one can

opt to a distributed relaxation partially decoupling the linear system associated with operator \mathbf{L} (2.16). In particular, the distribution matrix

$$(4.8) \quad \mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & -\frac{1}{\rho}\partial_x & 0 \\ 0 & 1 & 0 & -\frac{1}{\rho}\partial_y & 0 \\ 0 & 0 & 1 & -\frac{1}{\rho}\partial_z & 0 \\ \hat{\lambda}\partial_x & \hat{\lambda}\partial_y & \hat{\lambda}\partial_z & Q\frac{\hat{\lambda}+\mu}{\rho} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

results in

$$(4.9) \quad \mathbf{L}\mathbf{M} = \begin{bmatrix} Q\frac{\mu}{\rho} & 0 & 0 & 0 & 0 \\ 0 & Q\frac{\mu}{\rho} & 0 & 0 & 0 \\ 0 & 0 & Q\frac{\mu}{\rho} & 0 & 0 \\ \mathcal{P}\partial_x & \mathcal{P}\partial_y & \mathcal{P}\partial_z & QQ\frac{\hat{\lambda}+\mu}{\rho}c^2\Delta & (1-\gamma)\kappa\Delta \\ \frac{c^2}{\gamma}\partial_x & \frac{c^2}{\gamma}\partial_y & \frac{c^2}{\gamma}\partial_z & -\frac{c^2}{\gamma\rho}\Delta & Q\frac{\mu}{\rho} \end{bmatrix},$$

where $\mathcal{P} \equiv \rho c^2 + \hat{\lambda}Q$. The last two equations remain coupled, requiring a block 2-by-2 matrix solution in relaxation. This distributed relaxation scheme is still much less expensive than direct relaxation of matrix \mathbf{L} requiring solution for a block 5-by-5 matrix.

4.2. Traditional Factorizable Schemes. As mentioned previously, factorizability of a target discrete scheme significantly simplifies the distributed relaxation design. The main obstacle in this case to efficient solution is that the discretizations obtained for the scalar factors in the discrete determinant are not always convenient.

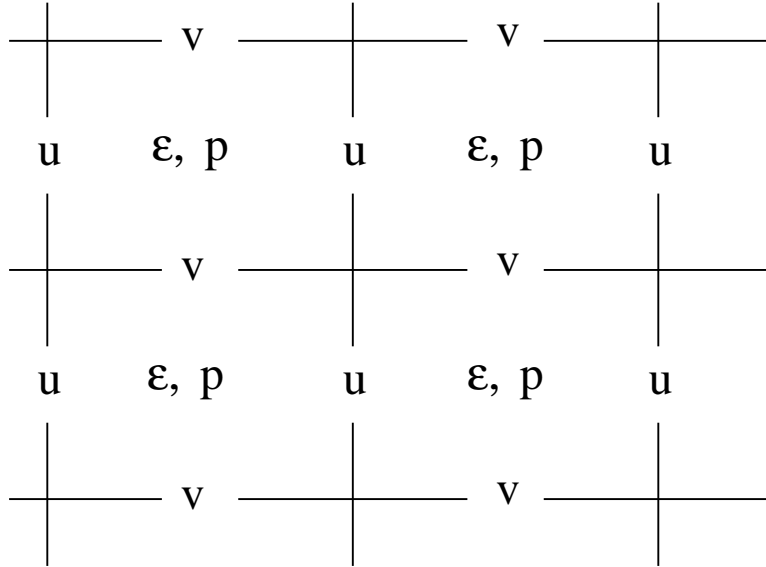


FIG. 4.1. *Staggered arrangement of primitive variables for Navier-Stokes discretization.*

4.2.1. Staggered-Grid Discretization for Navier-Stokes Equations. The staggered-grid discretization dating back to the mid 60's [27, 33, 34] is one of the first factorizable discretizations for incompressible flow equations. Compressible flow discretizations with a staggered arrangement of variables

have also been studied [29, 6, 52]. A usual placement of primitive variables in two dimensions is depicted in Figure 4.1. With this staggering, (a) the off-diagonal first derivatives in (3.2), (2.14), and (2.16) can be approximated as short central differences; (b) the second derivatives in (2.16) can be compositions of corresponding central first derivatives; (c) the convection-diffusion operators, Q_ν , can be approximated by any proper discretizations Q_ν^h . For discrete factorizability, it is important to have the same discretization for each of the Q_ν -operators in the momentum equations; the convection-diffusion operators in other equations can be different. The convection terms in the momentum and energy equations are usually upwind or upwind-biased; for simplicity, below we assume that all these terms are the same. With such differencing, the discrete schemes mimic the factorizability property of the differential equations, and the discrete system determinants can be factored as $\det \mathbf{L}^h = (Q_\nu^h)^2 \Delta^h$ (incompressible Navier-Stokes) or $\det \mathbf{L}^h = (Q^h)^3 (Q^h \bar{Q}^h - c^2 \Delta^h)$ (compressible Euler), where Δ^h in three dimensions is the seven-point h -Laplacian, Q^h is an upwind or upwind-biased discretization of the convection operators in the momentum and energy equations, \bar{Q}^h is a convection-operator discretization for the pressure term in the fourth equation of (2.14), hence $Q^h \bar{Q}^h - c^2 \Delta^h$ is a discrete approximation to the full-potential operator. The discrete determinant computed for the compressible Navier-Stokes equations is similar to the differential determinant (2.17).

The discrete distribution matrices follow directly from the continuous matrices (4.4), (4.6), and (4.8). The short central differences are used for the approximation of all the off-diagonal first derivatives; the convection parts in the Q -operators are the same as those in the momentum equations. The resulting products $\mathbf{L}^h \mathbf{M}^h$ are similar to those for the continuous problems with the main diagonals composed of the factors of the discrete determinants.

Distributed-relaxation solvers have been successfully applied to the staggered-grid discretization schemes for subsonic compressible [52] and incompressible [15, 53] flow problems.

In computing the Euler system of equations, the main disadvantages of the staggered-grid scheme relate to the discrete stencil of the full-potential operator. For subsonic flow problems, the downwind differencing applied for the \bar{Q}^h term results in a full-potential-operator stencil that is somewhat wide (because of the $Q^h \bar{Q}^h$ term) and poorly aligns with the physical (cross-stream) anisotropies in approaching the transonic regime. For supersonic flow, where the problem is purely hyperbolic, the stencil is not fully upwind (even if the \bar{Q}^h term is upwind differenced) implying more involved marching schemes.

Recently, a new approach to building discretization schemes that allows *any* desired differencing for the full-potential factor of the system determinant without compromising the scheme factorizability has been discovered. This approach is discussed subsequently in application to central collocated-grid discretizations (see also [26]), but it applies to staggered grids as well.

4.2.2. Collocated-Grid Discretizations for the Euler Equations. Another example of a factorizable scheme is a collocated-grid scheme with the second-order central differencing for the off-diagonal first derivatives in (3.2), (2.14), and (2.16). The convection operators in the momentum and energy equations are again upwind or upwind-biased; the differencing of the convection term applied to the pressure may alternate from downwind (downwind-biased) in subsonic mode to upwind (upwind-biased) in supersonic mode.

A typical difficulty associated with this type of schemes is a poor measure of h -ellipticity in the discrete approximation for the full-potential factor of the system determinant. To be more specific, let us define the

collocated-grid discretization \mathbf{L}^h of the matrix operator (2.14) as

$$(4.10) \quad \mathbf{L}^h = \begin{bmatrix} Q^h & 0 & 0 & \frac{1}{\rho} \partial_x^h & 0 \\ 0 & Q^h & 0 & \frac{1}{\rho} \partial_y^h & 0 \\ 0 & 0 & Q^h & \frac{1}{\rho} \partial_z^h & 0 \\ \rho c^2 \partial_x^h & \rho c^2 \partial_y^h & \rho c^2 \partial_z^h & \bar{Q}^h & 0 \\ \frac{c^2}{\gamma} \partial_x^h & \frac{c^2}{\gamma} \partial_y^h & \frac{c^2}{\gamma} \partial_z^h & 0 & Q^h \end{bmatrix},$$

where the discrete derivatives, $\partial_x^h, \partial_y^h, \partial_z^h$, in all off-diagonal terms are the wide (with mesh spacing $2h$) second-order-accurate central-differencing approximations. All the diagonal terms, Q^h , except \bar{Q}^h in the fourth equation, are discretized with the same second-order-accurate upwind (or upwind-biased) discretization scheme. In the subsonic regime ($|\mathbf{u}|^2 = \bar{u}^2 + \bar{v}^2 + \bar{w}^2 < c^2$), the \bar{Q}^h -term is discretized with a second-order-accurate downwind (or downwind-biased) discretization. The determinant of the matrix operator \mathbf{L}^h is given by

$$(4.11) \quad \left(Q^h\right)^3 \left[Q^h \bar{Q}^h - c^2 \Delta^{2h}\right],$$

where Δ^{2h} is a wide discretization of the Laplace operator. The full-potential-operator approximation appearing in the brackets has two major drawbacks: (1) For subsonic velocities ($|\mathbf{u}| < c$), the discrete operator is not h -elliptic, and efficiency of *any* local relaxation severely degrades. (2) For near-sonic regimes (the Mach number $M = |\mathbf{u}|/c \approx 1$), the discrete operator stencil does not reflect the physical anisotropies of the differential full-potential operator; the discrete operator exhibits a very strong coupling in the streamwise direction, while the differential operator has strong coupling only in the cross-stream directions.

Several approaches to cure the lack of h -ellipticity (mainly in applications to incompressible-flow equations) have been proposed in the literature (e.g., [1, 13]). Some of the approaches are associated with the introduction of additional terms increasing the measure of h -ellipticity in the system of equations, others propose averaging (filtering) spurious oscillations. The problem of wrong anisotropies in the full-potential-operator has not been sufficiently investigated. In two dimensions, it is possible to construct a discretization that satisfies the following properties: (1) At low Mach numbers, the discretization is dominated by the standard (with mesh spacing h) h -elliptic Laplacian. (2) For the transonic Mach numbers, the discretization tends to the optimal discretization [10, 11, 21] for the sonic-flow full-potential operator. (3) For supersonic Mach numbers, the discretization becomes upwind (upwind-biased) and can be solved by marching. The problem of constructing a good high-order discretization for the transonic full-potential operator in three dimensions is still open.

4.3. Non-Factorizable schemes. The majority of discrete schemes in current use, especially for compressible flow but also more recently for incompressible flow, are based upon a flux-splitting approach. The basis of this approach is the solution of the Riemann problem (i.e., the time evolution of two regions of flow initially separated by a diaphragm) applied on a dimension by dimension basis. This methodology has enabled the robust treatment of flows with strong shocks and complex geometries. However, the derived schemes are not discretely factorizable, except in one dimension.

These discrete equations have always been solved using collective relaxation (or pseudo-time-stepping) in multidimensional multigrid algorithms. A better efficiency should be realizable with a relaxation scheme that efficiently reduces both the high-frequency and characteristic error components. Such a scheme should combine two different relaxation methods: (1) A relaxation scheme treating directly the conservation equations and reducing the high-frequency error components. (2) A defect-correction (or predictor-corrector)

method with a factorizable driver (predictor) reducing characteristic error components. This approach has not been tried as yet.

4.4. Boundary Treatment. Boundaries and discontinuities introduce some additional complexity in distributed relaxation. The determinant of \mathbf{LM} is usually higher order than the determinant of \mathbf{L} . Thus, as a set of new variables, $\delta\mathbf{w}$ would generally need additional boundary conditions. In relaxation, because the ghost variables can be added in the external part of the domain, it is usually possible to determine suitable boundary conditions for $\delta\mathbf{w}$ that satisfy the original boundary conditions for the primitive variables.

Distributed relaxation is applied throughout the entire computational domain having the full effect away from boundaries (considering discontinuities as a special boundary case) in the regular (smoothly varying) flow field. The discrete equations near the boundaries are usually different from the interior equations; the relaxation equations are coupled near the boundaries, not decoupled as they are in the interior of the domain. Thus, some local procedures should supplement the distributed relaxation pass. The coupled near-boundary equations can be separated from other equations and solved (relaxed) with an appropriate method, such as direct solution or block-Newton-Kacmarcz relaxation. The additional work will not seriously affect the overall complexity because the number of boundary and/or discontinuity points is usually very small in comparison with the number of interior points.

Solution (or extensive relaxation) of the coupled near-boundary equations serves for two purposes. The first is to provide convenient and reliable boundary conditions for the distributed-relaxation equations in the interior. The second purpose arises because in the outer multigrid cycle, efficient fine-to-coarse grid restriction of residuals near the boundaries is difficult to design; it depends on many factors such as the shape of the boundary, the type of the boundary conditions, etc., and differs from the residual restriction in the interior. A general way to avoid efficiency degradation is to reduce residuals near the boundaries before restriction to a level that is significantly below the residual level characterizing the interior field. Having small residuals near the boundaries makes the precise form of the restriction operator less important.

5. Relaxation of Scalar Factors. Efficiency of the multigrid solvers exploiting factorizability of the Navier-Stokes system of equations is determined by the efficiency of the relaxation (solution) schemes applied for scalar factors appearing in the system determinant. For uniformly elliptic operators such as a Laplacian, a diffusion-dominated convection-diffusion operator, and a subsonic full-potential operator many efficient relaxation techniques are available (see textbooks [6, 17, 55, 56]). For such operators, an important relaxation requirement is efficient reduction of high-frequency errors. All the smooth components are well approximated on coarse grids built by standard (full) coarsening; therefore, the coarse-grid correction is efficient in reduction of smooth errors. For nonelliptic and weakly elliptic factors, e.g., convection, convection-dominated convection-diffusion, transonic and supersonic full-potential operators, (smooth) characteristic components cannot be approximated with standard multigrid methods [4, 10, 11, 15, 22].

Several approaches aimed at curing the characteristic-component problem have been studied in the literature. These approaches fall into two categories: (1) development of a suitable relaxation scheme (single-grid method) to eliminate not only high-frequency error components but the characteristic error components as well; (2) devising an adjusted coarse-grid operator to approximate well the fine-grid characteristic error components.

5.1. Single-Grid Methods.

5.1.1. Downstream marching. For hyperbolic problems, the simplest first-category method is downstream marching. If the corresponding discretization is a stable upwind discretization and the characteristic

field does not recirculate, then downstream marching is a very efficient solver that yields an accurate solution to a *nonlinear* hyperbolic equation in just a few sweeps (a single downstream sweep provides the exact solution to a linearized problem). The downstream marching technique was successfully applied in solving many CFD problems associated with non-recirculating flows (see, e.g., [15, 37, 45, 52, 53]). However, if a discretization operator is not fully upwind (e.g., is only upwind biased), straightforward downstream marching is unstable. For the schemes that cannot be directly marched, there are two possible alternatives (also of marching type): defect-correction and predictor-corrector methods.

5.1.2. Defect Correction. Let us consider a defect correction method for a discretized hyperbolic equation

$$(5.1) \quad L^h u_{i_1, i_2} = f_{i_1, i_2},$$

with specified inflow boundary conditions u_{0, i_2} .

Let \tilde{u}_{i_1, i_2} be the current solution approximation. Then the improved approximation \bar{u}_{i_1, i_2} is calculated by defect-correction scheme in the following two steps:

1. The correction v_{i_1, i_2} is calculated by solving operator L_d^h with a right-hand side represented by the residual of (5.1) computed for the current approximation \tilde{u}_{i_1, i_2} . The inflow boundary conditions for v are initialized with the zero values.

$$(5.2) \quad L_d^h v_{i_1, i_2} = f_{i_1, i_2} - L^h \tilde{u}_{i_1, i_2}.$$

2. The current approximation is corrected as

$$(5.3) \quad \bar{u}_{i_1, i_2} = \tilde{u}_{i_1, i_2} + v_{i_1, i_2}.$$

The operator L_d^h is called the *driver* operator. It is chosen to be easily solvable and usually less accurate than the target operator L^h ; the latter can be very general. If the iteration converges, steps (5.2) and (5.3) can be repeated until the desired accuracy is reached. Usually the efficiency of defect-correction methods is quite satisfactory [3, 19, 31, 52, 53], even though in principle the convergence rate of a defect-correction method for nonelliptic operator is normally mesh-size dependent [7, 23], as explained below.

In several papers (e.g., [19, 51]), authors studying the defect-correction method for nonelliptic problems observed a slow convergence or even a divergence in some common error norms for the initial iterations and good asymptotic convergence rates afterward. This behavior is different from that observed in solving elliptic problems by the defect-correction method, where the asymptotic convergence rate is the slowest one. This nonelliptic feature is explained by some properties associated with the cross-characteristic interaction (e.g., dissipation and/or dispersion) in the operators involved in the defect-correction iterations. Specifically, this cross-characteristic interaction defines the *penetration distance* (also termed “survival distance” [15]) of a characteristic component. The penetration distance is the distance from the inflow boundary within which the discrete solution of the homogeneous problem reasonably approximates the continuous one (i.e., the discretization error is substantially smaller than the solution).

The penetration distance of a characteristic component is roughly proportional to $\omega^{-1}(\omega h)^{-\frac{p}{q}}$, where q is the highest order of differentiation in the hyperbolic operator under considerations, p is the discrete-operator approximation order, ω is the cross-characteristic frequency of the characteristic component, and h is the mesh size. The ratio of penetration distances of the operators L^h and L_d^h is an important factor for determining the number of defect-correction sweeps required to reduce the algebraic error to the discretization-error level or to reach the asymptotic convergence regime.

When the operators L^h and L_d^h have the same approximation order ($p = r$), efficiency of the defect-correction method is optimal and mesh-size h -independent. If however the operators L^h and L_d^h have different approximation orders (p and r , respectively, $p > r$), then efficiency of the defect-correction method is h -dependent; i.e., the maximal number of sweeps which might be required to reduce the algebraic error to the discretization-error level (or to reach the asymptotic convergence rates) is larger on fine grids than on coarse grids. This is because one has to iterate L_d^h as many times as needed to attain accuracy up to the L^h penetration distance. The worst (largest) ratio of penetration distances is obtained for characteristic components for which the penetration distance in the target p -order accurate discretization approaches the depth R of the computational domain in the characteristic direction. It follows that the required number of iterations is proportional to $\left(\frac{R}{h}\right)^{\frac{p-r}{p+q}}$.

5.1.3. Predictor-Corrector. One potentially efficient but yet unexploited method to overcome grid-dependent convergence experienced in defect-correction iterations is the predictor-corrector technique. A detailed look into the defect-correction iteration reveals that the computational work distribution is unbalanced: (1) Driver operator iterations at locations beyond the penetration distance do not improve the solution approximation. (2) In successive iterations, the solution approximation near the inflow boundary becomes much more accurate than in the interior; the computational efforts spent in this regions could be more profitably invested at the accuracy frontier.

The predictor-corrector method has been extensively used for ordinary and time-dependent differential equations [18, 28]; however, applications for steady-state nonelliptic problems have been very limited. In predictor-corrector schemes, the final update of the solution at a particular point is computed from the local solution of the target operator. The solution values at downstream points included in the target-operator stencil are predicted from the solution of the driver (predictor) operator. In order to define a family of predictor-corrector schemes, one can divide the computational domain into several time-like layers; the first layer contains all the grid points adjacent to the inflow boundary. Each next layer is composed of the grid points that contribute to the stencils of target operators defined at the points of the previous layer and do not belong to any of the previous layers.

Now, a family of predictor-corrector schemes for solving the correction equation

$$(5.4) \quad L^h v_{i_1, i_2} = R_{i_1, i_2}^h \equiv f_{i_1, i_2} - L^h \tilde{u}_{i_1, i_2},$$

where L^h is the target operator, \tilde{u}_{i_1, i_2} is the current solution approximation with residual R_{i_1, i_2}^h , and v_{i_1, i_2} is the desired correction function, can be defined as

PC_0 : The solution of (5.4) is approximated by solving

$$(5.5) \quad L_d^h v_{i_1, i_2} = R_{i_1, i_2}^h.$$

This scheme is identical with the defect-correction scheme.

PC_k : Recursive definition of the derived predictor-corrector schemes (recursion with respect to k) can be done as follows: Assume the $(j-1)$ -th layer have already been finally updated in the current sweep. Then, to calculate new values at the next j -th layer one has to perform the following three steps:

1. To predict values at the j -th layer with PC_{k-1} scheme.
2. To predict values at the $(j+1)$ -th layer with PC_{k-1} scheme.
3. To update values at the j -th layer by directly relaxing (5.4).

The schemes for $k = 0, 1, 2$ have been tested for a linearized supersonic full-potential operator [21].

5.2. Multigrid methods.

5.2.1. Recirculation. Downstream marching methods are not viable for problems with closed characteristics. Alternative discretization and solution techniques should be considered. The discretization issue becomes especially important for flows with streamlines that do not start and end at boundaries, but constitute closed curves. In such cases, even a very small viscosity plays an important role in determining the flow throughout the domain. The solution in the limit of vanishing viscosity depends very strongly on how the viscosity coefficients tend to zero. The propagation of information from the boundary into the domain is governed by the viscous terms no matter how small they may be. It has been shown [14] for both the scalar convection-diffusion problem and the incompressible Navier-Stokes equations that varying cross-stream numerical viscosity (caused usually by varying angles between the stream and the grid lines; e.g., in standard upwind and upwind biased schemes) may prevent convergence to a physically realizable solution. In the most general case, it can be shown that even isotropic viscosity is not sufficient for convergence to a physical solution, and one must actually specify a *uniform* viscosity. However, for the homogeneous problems there are several indications [14, 59] (though no proof) that isotropy suffices.

To obtain a discretization scheme that exhibits the appropriate physical-like behavior for vanishing viscosity, one must either add sufficient explicit isotropic viscosity that will dominate the anisotropic numerical viscosity of the convection operator, or else derive a discrete convection operator with numerical viscosity satisfying the condition of isotropy. An upwind isotropic-viscosity discretization has been derived [59].

One general approach to the algebraic solution of nonelliptic equations with closed characteristics is to apply a multigrid method with an overweighted upwind-biased residual restriction. Efficient multigrid solvers for recirculating convection equation have already been demonstrated [16, 59]. This approach is well combined with the distributed relaxation method for the Navier-Stokes equations, because within a distributed relaxation sweep a multigrid solver with optimal overweighting can be applied to a separate scalar nonelliptic equation with closed characteristics.

Another solution approach is to apply some general techniques to approximate indirectly smooth characteristic components. Among helpful techniques are recombination of iterants, cycles with high indexes, and implicit alternative-direction relaxation. Recombination of iterants (solution approximations on different stages of a multigrid algorithm) at each grid level eliminates several (number of iterants minus one) error components, those, more specifically, that are most prominent in the residual function. Making increasingly many coarse-grid iterations per each fine-grid iteration, cycles with high indexes solve the characteristic-component problem on coarser grids. Implicit alternative-direction relaxation simulates downstream marching in the regions with open characteristics and efficiently transfers information in the regions with characteristics closely aligned with the grid. Theoretically, each of these methods cannot completely resolve the problem of poor coarse-grid correction to the fine-grid smooth characteristic error components. The problem already manifests itself in two-level algorithms with any type of local relaxation. On fine grids the number of problematic error components may increase, and many cycles may be needed to collect the necessary number of the fine-grid iterants to exclude all the troubling error components. However, it has been shown experimentally [32] that a combination of implicit alternative-direction defect-correction type relaxation, recombination of iterants on all the levels, and W-cycles can result in a relatively efficient multigrid solver for recirculating flow problems on practical grids.

5.2.2. Full-Potential Operator. The full-potential operator is a variable type operator, and its solution requires different procedures in subsonic, transonic, and supersonic regions. In deep subsonic regions, the full-potential operator is uniformly elliptic and therefore standard multigrid methods yield optimal

efficiency. When the Mach number approaches unity, the operator becomes increasingly anisotropic and, because smooth characteristic error components cannot be approximated adequately on coarse grids, classical multigrid methods severely degrade. In the deep supersonic regions, the full-potential operator is uniformly hyperbolic with the stream direction serving as the time-like direction. In this region, an efficient solver can be obtained with a downstream marching method. However, downstream marching becomes problematic for the Mach number dropping towards unity, because the Courant number associated with this method becomes large. Thus, a special procedure is required to provide an efficient solution for transonic regions. A possible local procedure [10, 11, 20, 21] is based on piecewise semicoarsening and some rules for adding dissipation at the coarse-grid levels.

A similar technique can be used to construct an efficient marching-free multigrid solver for convection-dominated equations. This method [22] employs a colored relaxation scheme and is very attractive for massive parallel computing. A highly parallel multigrid solver for the supersonic full-potential operator may be obtained by methods similar to the wave/ray multigrid [12].

6. Analysis. As mentioned previously, it is important in attaining optimal efficiency to understand all the difficulties that present themselves in application. Analysis methods are quite helpful in this regard, and the main tools are discussed below. In iterative methods solving elliptic problems, the main mechanism of convergence is damping of error components. In solution of hyperbolic scalar equations, there is another very important convergence mechanism: the downstream evolution of the error components. In the presence of this additional mechanism, the accuracy first achieved near the inflow boundary and is then propagated into the interior of the domain.

The recognition of this additional convergence mechanism urges modifications in the standard analysis developed for elliptic problems. Basically, one can distinguish four types of analysis applied to nonelliptic problems: (1) standard linear-algebraic matrix analysis, (2) modified zero-mode-exclusion full-space Fourier mode analysis, (3) half-space analysis of the first differential approximations (FDA) [4, 57, 58], and (4) discrete half-space analysis. Briefly, the first differential approximation (also called modified equation) to a difference operator on a grid with mesh size h is the Taylor expansion of this difference operator in terms of h truncated to the first terms including the least nonzero power of h . The quality of an analysis applied to nonelliptic problems is determined by how well the analysis handles the characteristic components.

6.1. Matrix analysis. The most general and precise analysis methods are the linear-algebra matrix analysis methods applied to the corresponding linearized problem. This analysis considers the difference operators without assumptions about the solution and boundary conditions. It can be applied to variable-coefficient problems as well. This analysis was found very useful for analyzing one-dimensional problems. However, the enormous computational complexity of this analysis makes it not viable for multidimensional problems. Although, the analysis complexity can be reduced considerably by assuming Fourier modes in two of the three spatial directions.

6.2. Modified full-space Fourier mode analysis. The modified full-space Fourier mode analysis is a modification of the standard full-space Fourier mode analysis excluding from the consideration all the zero modes (the modes with vanishing symbols) [56]. It is the simplest and most popular type of analysis (e.g., see applications in [19, 31]). This analysis estimates only the amplification (damping) factor. Its inherent disadvantage is the inability to take the influence of the inflow boundary into account. This explains its failure in describing the downstream error evolution. However, the modified full-space analysis can also be useful for analyzing the effect of forcing terms.

6.3. FDA half-space analysis. The FDA half-space analysis is a relatively simple and efficient tool for analyzing the effect of the inflow boundary. Examples of applications of this analysis are available [4, 15, 57, 58]. The first differential approximations are considered on a half-space including an inflow boundary. The boundary conditions are represented by one Fourier mode at a time. The FDA analysis provides a good *qualitative* description of the downstream error evolution. This analysis focuses on characteristic components and, therefore, considers homogeneous problems. Note that a combination of the FDA analysis with the modified full-space analysis can provide a good insight for nonhomogeneous problems as well. The disadvantages of this analysis are the inability to provide quantitative estimates, to analyze the effect of different boundary condition discretizations, and to address the asymptotic convergence rate.

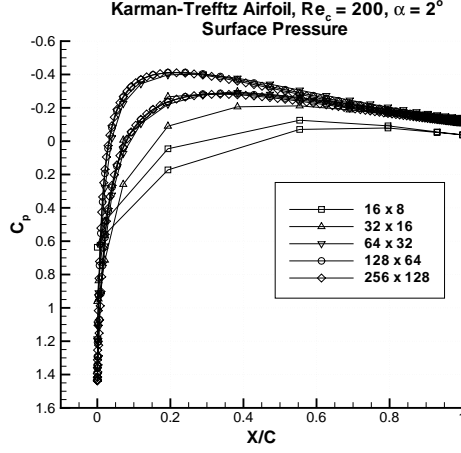
6.4. Discrete half-space analysis. The discrete half-space analysis [10, 23] considers the discretizations in their exact form rather than their differential approximation, while the boundary data are represented by a Fourier component. This analysis translates the original multidimensional problem into a one-dimensional discrete problem, where the frequencies of the boundary Fourier components are considered as parameters. To regularize the half-space problem, the solution is not allowed to grow faster than a polynomial function. This tool is very accurate; it can be used to explain in detail many phenomena observed in solving nonelliptic equations and provides a close prediction of the actual solution behavior.

The one-dimensional solution obtained in the discrete half-space analysis has two different representation forms: (1) away from the boundary, the solution is defined as a linear combination of a finite number of analytical components; this region is called the *analytical representation region*; (2) in the region adjacent to the inflow boundary, the solution is defined pointwise; this zone is referred to as the *pointwise representation region*. With each further iteration described by the analysis, the pointwise representation region penetrates by a finite number of mesh sizes into the interior. By using these representations, the computational complexity of the analysis becomes much less than that associated with the one-dimensional matrix analysis. In the asymptotic regime, when the pointwise representation zone covers all the domain, this analysis becomes a discrete one-dimensional matrix analysis of the multidimensional problem.

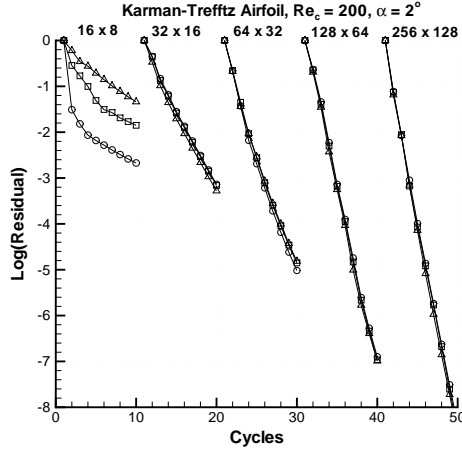
The discrete half-space analysis provides a *quantitative* description of the approximate solution; it predicts the convergence rate for each iteration and the asymptotic convergence rate. It can be easily adjusted to analyze the global effect of *any* local discretization of the inflow boundary conditions. This adjustment can be done just by widening the initial pointwise representation region at the inflow boundary. If necessary, the analysis can take into account the influence of the discretized *outflow* boundary conditions as well. Generally, this discrete half-space analysis treats completely both mechanisms of convergence, damping and downstream evolution of errors, associated with nonelliptic problem solvers.

7. Summary of Recent Progress.

7.1. Pressure-Equation Discretization. The original pressure-equation formulation [45] has been extended to general coordinates and implemented for lifting airfoils in inviscid flow [36, 37, 39] and viscous flow [47]. The results for viscous flow over a lifting airfoil at low Reynolds number are shown in Figure 7.1. An alternating line-implicit Gauss-Seidel relaxation is used to treat the mesh anisotropy that generally occurs in resolving viscous boundary layers on stretched grids. The computed pressure distributions are nearly indistinguishable from each other on the finer grids. The convergence rate actually becomes better as grids are refined and more levels in the FAS cycle are used; the 16x8 grid is always the coarsest grid in the multigrid computations. The convergence rates are comparable to the rates obtained for fully elliptic problems.



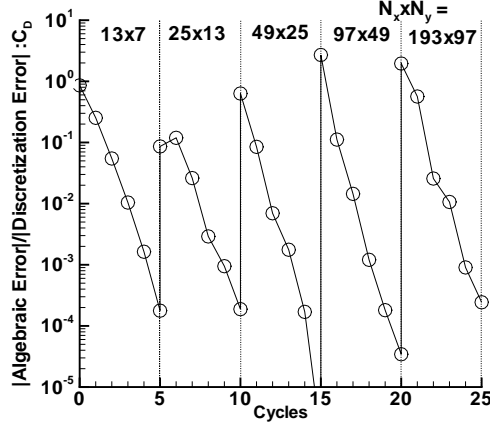
(a) Pressure distribution on the upper and lower surfaces for a sequence of grids.



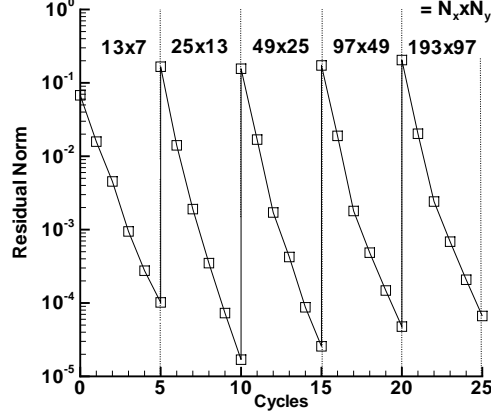
(b) Residual convergence with an FMG method using 10 FAS cycles on each grid from the coarsest 16x8 to the finest 256x128 (squares: x -momentum; triangles: y -momentum; circles:pressure equation).

FIG. 7.1. Computational results for the incompressible viscous flow over a lifting Kármán-Trefftz airfoil at $Re = 200$ and $\alpha = 2^\circ$.

7.2. Staggered-Grid Factorizable Discretization. The first TME solver applying the distributed relaxation approach for solution to an entering flow problem for the incompressible Navier-Stokes equations was developed using a staggered-grid formulation [15]. This formulation was extended to the compressible NS equations and fast convergence rates were demonstrated [52] for several viscous model problems. This latter work was the first experience with distributed relaxation in the computation of compressible viscous flows in which a 2×2 block was relaxed simultaneously in line-implicit Gauss-Seidel relaxation. The coupling of boundary and interior relaxation was not optimally treated at the time. A more complete study on TME for the incompressible equations at high-Reynolds-number conditions has been recently performed [53]. In all calculations, a staggered arrangement of variables on Cartesian grids has been used. With distributed relaxation, the system of equations has been decomposed (i.e., factored) everywhere, except near boundaries where the equations remained coupled. The results of the calculation are shown in Figure 7.2 for the viscous flow over a finite flat plate. The convergence of residuals and the algebraic-to-discretization errors in drag



(a) Algebraic-to-discretization errors in drag, C_D .

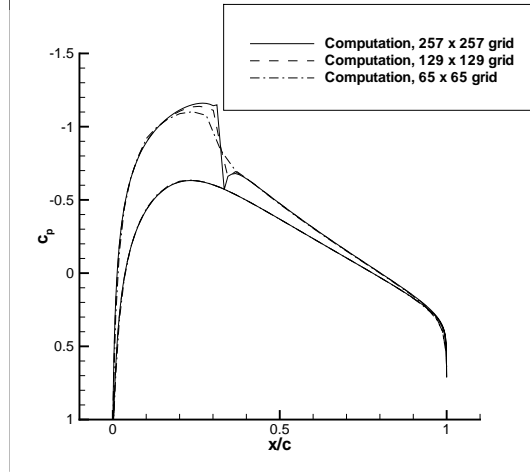


(b) L_2 -norm of the residual.

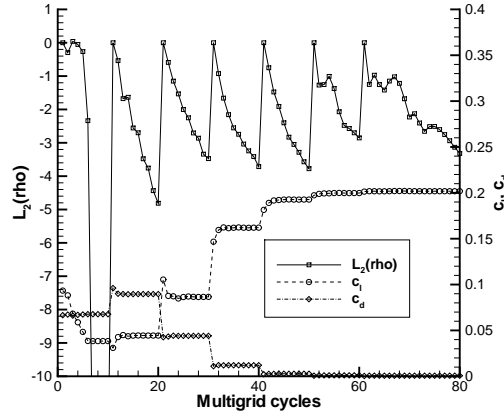
FIG. 7.2. Convergence of errors in an FMG cycle using 5 FAS cycles on each grid from the coarsest 13×7 to the finest 193×97 for the incompressible viscous flow over a flat plate at $Re = 10,000$.

are shown versus multigrid cycles. The residual convergence rate is about the same as for the underlying Laplacian factor. The FMG solver with just one FAS multigrid cycle per grid level and a total computational work equivalent to about 10 target-grid residual evaluations converged the drag to the discretization accuracy.

7.3. New Factorizable Collocated-Grid Discretizations. Recently, a new multidimensional factorizable scheme for the Euler equations has been developed [42] for Cartesian coordinates and extended through generalized coordinates to external lifting flows around airfoils with both subcritical and supercritical freestream Mach numbers [38, 35]. The starting point for the scheme is the first-order discretization of the flux-difference splitting scheme [40]. Correction terms are added in the form of mixed derivatives to make the scheme both second-order accurate and discretely factorizable. The resulting scheme is second-order accurate and compact in comparison to other scheme; it is the first flux-difference-splitting scheme that is discretely factorizable in multiple dimensions. Discrete factorizability is achieved by using some non-standard wide approximations for spatial derivatives to ensure that the identities



(a) Surface pressure (C_p) on a sequence of three grids.



(b) Convergence of residual and forces (lift and drag) in an FMG cycle with 20 FAS cycles on the finest 257×257 mesh and 10 FAS cycles on each coarser mesh.

FIG. 7.3. Computational results for compressible Euler flow over a lifting Kármán-Trefftz airfoil; $M_\infty = 0.70$; $\alpha = 1^\circ$.

$$\begin{aligned}\partial_{xx}\partial_{yy} &= \partial_{xy}\partial_{xy}, \\ \partial_{xx}\partial_y &= \partial_{xy}\partial_x, \\ \partial_{yy}\partial_x &= \partial_{xy}\partial_y\end{aligned}$$

are satisfied on the discrete level. The determinant of the resulting scheme is composed of an upwind differenced convection factor and an h -elliptic approximation for the full-potential factor. The distributed relaxation is possible by using a left and right distribution matrix, although this has not been applied as yet.

In numerical tests performed for this scheme, the multigrid solver employed symmetric point collective Gauss-Seidel relaxation. Computations for subsonic and transonic channel flows with essentially grid-independent convergence rates have been presented [38]. Grid-independent convergence rates have also been attained for a flow with stagnation points [35]. The convergence rates observed in experimenting with subsonic flow over a lifting airfoil were quite fast (about 0.3 per multigrid V-cycle) and only slightly grid dependent. The rates somewhat deteriorate in transonic/supersonic computations, emphasizing the need

for distributed relaxation. The scheme applies at low Mach numbers although it has yet to be extended to viscous flows. Multigrid results for the transonic flow over a lifting Kármán-Trefftz airfoil with a shock are shown in Figure 7.3. The pressure distribution shows the weak shock that is captured by the scheme. The residual convergence indicates some deterioration of the rate on the finer grids but the lift and drag coefficients are converged to below discretization error levels in only a few cycles.

Another approach to building factorizable schemes with suitable discretizations for scalar factors has been explored in papers of the second and third authors [24, 26, 25]. The approach is based on a collocated-grid scheme with a mechanism that allows one to improve the h -ellipticity measure by obtaining *any* desired discretizations for the full-potential factor of the system determinant without compromising the discrete factorizability. Also, the distribution matrices follow directly from the discrete forms for \mathbf{M} presented earlier. The same approach can be applied for incompressible-flow problems and to staggered-grid discretizations as well.

The starting point is the discretization (4.10). The way proposed to improve the discrete full-potential operator is to change the discretization of \bar{Q}^h to $\bar{Q}^h + \mathcal{A}^h$. Then the discrete full-potential operator is changed to

$$(7.1) \quad Q^h \mathcal{A}^h + Q^h \bar{Q}^h - c^2 \Delta^{2h},$$

where $\mathcal{A}^h = (Q^h)^{-1} \mathcal{D}^h$, $\mathcal{D}^h = \mathcal{F}^h - (Q^h \bar{Q}^h - c^2 \Delta^{2h})$, and \mathcal{F}^h is a desired approximation for the full-potential factor. In smooth regions, \mathcal{A}^h is second-order small (proportional to h^2), hence the overall second-order discretization accuracy is not compromised. The operator $(Q^h)^{-1}$ is a nonlocal operator and its introduction can be effected through a new auxiliary variable ψ^h and a new discrete equation $Q^h \psi^h = \mathcal{D}^h p^h$.

Thus, the corrected discrete approximation to (2.14) is defined as

$$(7.2) \quad \mathbf{L}^h = \begin{bmatrix} Q^h & 0 & 0 & 0 & \frac{1}{\rho} \partial_x^h & 0 \\ 0 & Q^h & 0 & 0 & \frac{1}{\rho} \partial_y^h & 0 \\ 0 & 0 & Q^h & 0 & \frac{1}{\rho} \partial_z^h & 0 \\ 0 & 0 & 0 & Q^h & -\mathcal{D}^h & 0 \\ \rho c^2 \partial_x^h & \rho c^2 \partial_y^h & \rho c^2 \partial_z^h & 1 & \bar{Q}^h & 0 \\ \frac{c^2}{\gamma} \partial_x^h & \frac{c^2}{\gamma} \partial_y^h & \frac{c^2}{\gamma} \partial_z^h & 0 & 0 & Q^h \end{bmatrix}.$$

The corresponding distribution matrix, \mathbf{M}^h , for distributed relaxation is defined as

$$(7.3) \quad \mathbf{M}^h = \begin{bmatrix} 1 & 0 & 0 & 0 & -\frac{1}{\rho} \partial_x^h & 0 \\ 0 & 1 & 0 & 0 & -\frac{1}{\rho} \partial_y^h & 0 \\ 0 & 0 & 1 & 0 & -\frac{1}{\rho} \partial_z^h & 0 \\ 0 & 0 & 0 & 1 & \mathcal{D}^h & 0 \\ 0 & 0 & 0 & 0 & Q^h & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

so that the resulting matrix $\mathbf{L}^h \mathbf{M}^h$ becomes lower triangular as

$$(7.4) \quad \mathbf{L}^h \mathbf{M}^h = \begin{bmatrix} Q^h & 0 & 0 & 0 & 0 & 0 \\ 0 & Q^h & 0 & 0 & 0 & 0 \\ 0 & 0 & Q^h & 0 & 0 & 0 \\ 0 & 0 & 0 & Q^h & 0 & 0 \\ \rho c^2 \partial_x^h & \rho c^2 \partial_y^h & \rho c^2 \partial_z^h & 1 & \mathcal{F}^h & 0 \\ \frac{c^2}{\gamma} \partial_x^h & \frac{c^2}{\gamma} \partial_y^h & \frac{c^2}{\gamma} \partial_z^h & 0 & -\frac{c^2}{\gamma \rho} \Delta^{2h} & Q^h \end{bmatrix}.$$

The scheme as defined above is valid for nonconservative flows. A version to be used for distributed relaxation of conservative equations has also been designed [24].

Numerical tests have only been performed as yet for a quasi-one-dimensional subsonic flow in a convergent/divergent channel. The accuracy was comparable to other schemes. With proper treatment of the distributed-relaxation equations in the regions adjacent to the boundaries, the convergence of the multigrid solver with a V-cycle and two relaxation sweeps per level is identical with the convergence of a similar multigrid solver for the discrete full-potential operator.

8. Concluding Remarks. Fundamentals and recent advances towards the development of TME solvers for fluid simulations have been presented. Accurate discrete approximations to the solution of the differential equations are obtained with FMG methods through fast reduction of algebraic errors below the discretization error level on each mesh. Strategies to attain TME for general fluid systems by exploiting factorizability of the governing differential equations are reviewed. These strategies include a reformulation of the target differential equations and a distributed relaxation approach applied to the original equations. New discretizations and computations demonstrating this methodology for inviscid and viscous flow simulations have been presented.

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